

Accuracy of the diffusion equation with extrapolated-boundary condition for transmittance of light through a turbid medium

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The linear intensity profile of multiply scattered light in a slab geometry extrapolates to zero at a certain distance beyond the boundary. The diffusion equation with this “extrapolated boundary condition” has been used in the literature to obtain analytical formulas for the transmittance of light through the slab as a function of angle of incidence and refractive index. The accuracy of these formulas is determined by comparison with a numerical solution of the Boltzmann equation for radiative transfer.

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I. INTRODUCTION

Multiple scattering of light in a turbid medium is well described by the theory of radiative transfer [1, 2, 3]. This theory is based on a Boltzmann equation for the stationary intensity $I(\vec{r}, \hat{s})$ of monochromatic light at position \vec{r} and with wave vector in the direction \hat{s} . In the simple case of isotropic and non-absorbing scatterers (with mean free path l), the Boltzmann equation takes the form

$$l \hat{s} \cdot \vec{\nabla} I(\vec{r}, \hat{s}) = -I(\vec{r}, \hat{s}) + \bar{I}(\vec{r}). \quad (1)$$

Far from boundaries the angle-averaged intensity, given here for 3 dimensions,

$$\bar{I}(\vec{r}) \equiv \int \frac{d\hat{s}}{4\pi} I(\vec{r}, \hat{s}) \quad (2)$$

satisfies the diffusion equation

$$\nabla^2 \bar{I}(\vec{r}) = 0, \quad (3)$$

which is easier to solve than the Boltzmann equation. The diffusion equation breaks down within a few mean free paths from the boundary, and one needs to return to the Boltzmann equation in order to determine $\bar{I}(\vec{r})$ near the boundaries.

A great deal of work has been done on the choice of boundary conditions for the diffusion equation which effectively incorporate the non-diffusive boundary layer [1, 2, 4, 5, 6, 7, 8]. These studies have led to the so called “extrapolated-boundary condition”

$$\bar{I}(\vec{r}) = -\xi \hat{n} \cdot \vec{\nabla} \bar{I}(\vec{r}), \quad (4)$$

where \vec{r} is a point on the boundary and \hat{n} is a unit vector perpendicular to the boundary and pointing outwards. Equation (4) implies that a linear density profile extrapolates to zero at a distance ξ beyond the boundary. The extrapolation length ξ is of the order of the mean free path.

In this paper we consider transmission through a slab of finite thickness L . We compute the transmittance

T , the ratio between the incident flux and the transmitted flux, by solving the Boltzmann equation numerically. Previous work on this problem used the diffusion equation with the extrapolated-boundary condition [9, 10, 11, 12] (or an alternative large- L/l approximation [7]) to derive convenient analytical formulas for the dependence of T on L and l , on the refractive index of the slab, and on the angle of incidence. It is the purpose of the present study to determine the accuracy of these formulas, by comparison with the results from the Boltzmann equation. We generalize and extend a previous study by De Jong [13] in the context of electrical conduction through a disordered metal, where the issue of refractive-index mismatch and angular resolution has not been considered.

II. CALCULATION OF THE TRANSMITTANCE FROM THE BOLTZMANN EQUATION

We consider a slab containing a disordered medium between the planes $z = 0$ and $z = L$ (see Fig. 1). The intensity $I(\vec{r}, \hat{s})$ depends only on the z -coordinate and on the angle θ between \hat{s} and the z -axis. We define $\mu \equiv \cos \theta$. The Boltzmann equation (1) takes the form

$$l\mu \frac{\partial}{\partial z} I(z, \mu) = -I(z, \mu) + \bar{I}(z), \quad 0 < z < L, \quad (5a)$$

$$\bar{I}(z) = \frac{1}{2} \int_{-1}^1 d\mu I(z, \mu). \quad (5b)$$

We supplement Eq. (5) with boundary conditions at $z = 0$ and $z = L$ that describe reflection due to a refractive index mismatch, with reflection probability $R(\mu)$:

$$I(0, \mu) = R(\mu)I(0, -\mu) + I_0(\mu), \quad \mu > 0, \quad (6a)$$

$$I(L, -\mu) = R(\mu)I(L, \mu). \quad \mu > 0, \quad (6b)$$

The boundary condition at $z = 0$ also contains the intensity due to a planar source with angular distribution

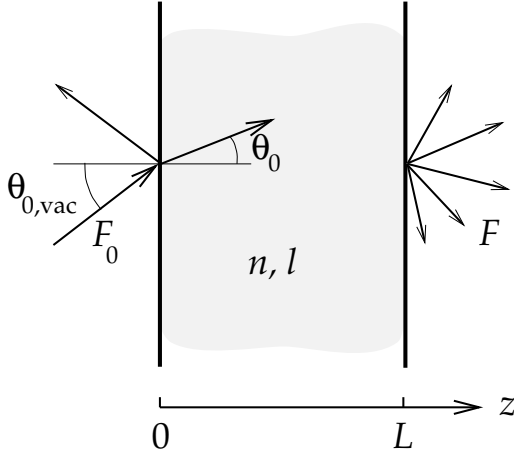


FIG. 1: A sketch of the slab geometry. The disordered medium (thickness L) has a refractive index n (relative to the outside) and a mean free path l . The slab is illuminated by a plane wave incident at an angle $\theta_{0,\text{vac}}$, which is refracted to an angle θ_0 inside the medium. The transmittance T is the ratio of the transmitted flux F and the incident flux F_0 .

$I_0(\mu)$ inside the medium. Note that the angular distribution is different from that outside the medium, due to refraction at the boundary and due to the fact that part of the light is reflected before even entering the medium.

The Boltzmann equation (5) with boundary conditions (6) implies for $\bar{I}(z)$ an integral equation of the Schwarzschild-Milne type [1, 6, 7, 13]

$$\begin{aligned} \bar{I}(z) = & M_0(z) + \int_0^L dz' \bar{I}(z') \left[M_1(z-z') + \right. \\ & M_2(z+z') + M_2[(L-z) + (L-z')] + \\ & \left. M_3(z-z') + M_3[(L-z) - (L-z')] \right]. \end{aligned} \quad (7)$$

We have defined the kernels

$$M_1(z) = \int_0^1 \frac{d\mu}{2l\mu} e^{-|z|/l\mu}, \quad (8a)$$

$$M_2(z) = \int_0^1 \frac{d\mu}{2l\mu} N(\mu) R(\mu) e^{-z/l\mu}, \quad (8b)$$

$$M_3(z) = \int_0^1 \frac{d\mu}{2l\mu} N(\mu) R^2(\mu) e^{-(2L+z)/l\mu}. \quad (8c)$$

The factor N is given by

$$N(\mu) = \left(1 - R^2(\mu) e^{-2L/l\mu} \right)^{-1}. \quad (9)$$

The kernels M_1 , M_2 , and M_3 describe propagation from z' to z with zero, an odd number, and an even number of reflections, respectively. The source term M_0 is given by

$$M_0(z) = \frac{1}{2} \int_0^1 d\mu N(\mu) I_0(\mu) \left[e^{-z/l\mu} + R(\mu) e^{-(2L-z)/l\mu} \right]. \quad (10)$$

Once $\bar{I}(z)$ is known, the intensities $I(z, \mu)$ and $I(z, -\mu)$ with $\mu > 0$ follow from

$$\begin{aligned} I(z, \mu) = & I_0(\mu) N(\mu) e^{-z/l\mu} + \int_0^z \frac{dz'}{l\mu} e^{(z'-z)/l\mu} \bar{I}(z') \\ & + N(\mu) R(\mu) e^{-z/l\mu} \\ & \times \int_0^L \frac{dz'}{l\mu} \left(e^{-z'/l\mu} + R(\mu) e^{-(2L-z')/l\mu} \right) \bar{I}(z'), \end{aligned} \quad (11a)$$

$$\begin{aligned} I(z, -\mu) = & I_0(\mu) N(\mu) R(\mu) e^{-(2L-z)/l\mu} \\ & + \int_z^L \frac{dz'}{l\mu} e^{(z-z')/l\mu} \bar{I}(z') \\ & + N(\mu) R(\mu) e^{-(2L-z)/l\mu} \\ & \times \int_0^L \frac{dz'}{l\mu} \left(e^{z'/l\mu} + R(\mu) e^{-z'/l\mu} \right) \bar{I}(z'). \end{aligned} \quad (11b)$$

This is a solution of the Boltzmann equation (5) with boundary conditions (6), as can be checked by substitution. Integration over all μ then yields the Schwarzschild-Milne equation (7). We solve the integral equation (7) numerically, by discretizing the interval $(0, L)$, so that it reduces to a matrix equation [13].

The quantity of interest is the transmittance T , defined as the ratio of the flux F that is transmitted through the slab and the flux F_0 incident from the source,

$$T = F/F_0. \quad (12)$$

The transmitted flux is given by

$$F = 2\pi \int_{-1}^1 d\mu \mu I(z, \mu), \quad (13)$$

where c is the speed of light in the medium. The flux is independent of z , because there is no absorption. The total incident flux (including the flux which is reflected at the slab boundary before entering the medium) is given by

$$F_0 = 2\pi \int_{\mu_c}^1 d\mu \frac{\mu I_0(\mu)}{1 - R(\mu)}. \quad (14)$$

We assume that the medium in the slab has a refractive index $n > 1$ (relative to the refractive index outside the slab). The lower bound μ_c in the integral, defined by $\mu_c \equiv (1 - 1/n^2)^{1/2}$, is the cosine of the angle at which total internal reflection occurs [$R(\mu) \equiv 1$ for $\mu < \mu_c$]. For $0 < \mu < \mu_c$ the reflection probability is given by the Fresnel formula for unpolarized light,

$$R(\mu) = \frac{1}{2} \left| \frac{\mu_{\text{vac}} - n\mu}{\mu_{\text{vac}} + n\mu} \right|^2 + \frac{1}{2} \left| \frac{n\mu_{\text{vac}} - \mu}{n\mu_{\text{vac}} + \mu} \right|^2, \quad (15a)$$

$$\mu_{\text{vac}} \equiv [1 - n^2(1 - \mu^2)]^{1/2}. \quad (15b)$$

The relation between $\mu_{\text{vac}} = \cos \theta_{\text{vac}}$ and $\mu = \cos \theta$ is Snell's law, such that the angle of incidence θ_{vac} outside

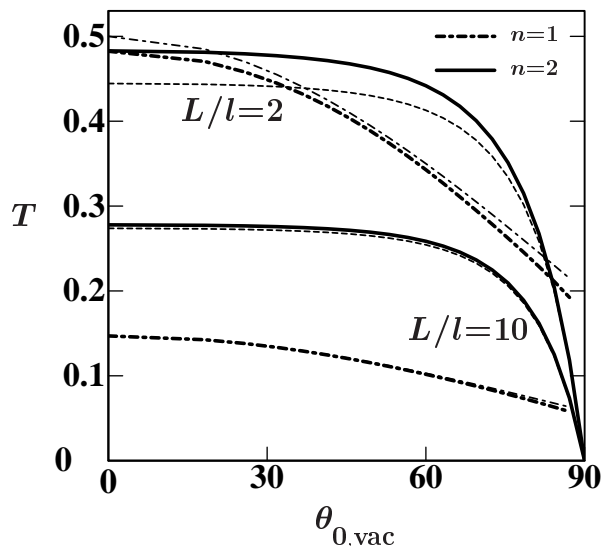


FIG. 2: Transmittance as a function of the incident angle $\theta_{0,\text{vac}}$ for two different values of L and n . The thick curves are computed from the Boltzmann equation, the thin curves are the diffusion approximation (20).

the medium (in “vacuum”) is refracted to an angle θ in the medium (see Fig. 1).

We have calculated the transmittance for the case of plane-wave illumination, $I_0(\mu) = I_0\delta(\mu - \mu_0)$. The results are shown in Fig. 2, where T is plotted as a function of the angle of incidence $\theta_{0,\text{vac}}$ outside the medium [$\mu_{0,\text{vac}} = \cos \theta_{0,\text{vac}}$ is related to μ_0 by Eq. (15b)]. We show results for two different ratios L/l and two values of n (thick curves). For $n = 1$ the transmittance is non-zero for all incident angles, but numerical difficulties prevent us from going beyond $\theta_{0,\text{vac}} \simeq 87^\circ$. The thin curves in Fig. 2 are the results of the diffusion approximation, which we discuss in the following section.

III. COMPARISON WITH THE DIFFUSION APPROXIMATION

The diffusion approximation for the transmittance has been studied by several authors [9, 10, 11, 12]. Here we briefly describe this approach, and then compare the result with the numerical solution of the Boltzmann equation.

In a slab geometry the diffusion equation with extrapolated-boundary condition takes the form [cf. Eqs. (3) and (4)]

$$\frac{d^2}{dz^2} \bar{I}(z) = 0, \quad 0 < z < L, \quad (16)$$

with boundary conditions

$$\bar{I}(0) = \xi \bar{I}'(0), \quad \bar{I}(L) = -\xi \bar{I}'(L). \quad (17)$$

We assume plane-wave illumination of the boundary $z = 0$, at an angle $\theta_{0,\text{vac}}$ with the positive z -axis. A fraction

$1 - R(\mu_0)$ of the incident flux F_0 enters the medium, and is first scattered on average at $z = \mu_0 l$. [We recall that $\mu_0 = \cos \theta_0$, where θ_0 corresponds to $\theta_{0,\text{vac}}$ after refraction, cf. Eq. (15b).] This plane-wave illumination is incorporated into the diffusion equation (16) as a source term,

$$\frac{d^2}{dz^2} \bar{I}(z) + \frac{3}{4\pi l} [1 - R(\mu_0)] F_0 \delta(z - \mu_0 l) = 0. \quad (18)$$

The solution of Eq. (18) with boundary condition (17) is

$$\bar{I}(z) = \begin{cases} \frac{3}{4\pi l} \frac{(\xi + z)(L + \xi - \mu_0 l)}{L + 2\xi} \times [1 - R(\mu_0)] F_0, & \text{if } 0 < z < \mu_0 l, \\ \frac{3}{4\pi l} \frac{(\xi + \mu_0 l)(L + \xi - z)}{L + 2\xi} \times [1 - R(\mu_0)] F_0, & \text{if } \mu_0 l < z < L. \end{cases} \quad (19)$$

The transmitted flux $F = -\frac{4}{3}\pi \bar{I}'(L)$ divided by the incident flux F_0 leads to the transmittance in the diffusion approximation,

$$T_{\text{diff}} = [1 - R(\mu_0)] \frac{\xi + \mu_0 l}{L + 2\xi}. \quad (20)$$

This simple analytical formula combines results in the literature by Kaplan et al. [9] (who considered normal incidence) and by Nieuwenhuizen and Luck [7] (who considered the Schwarzschild-Milne equation in the diffusive limit $L \gg l$).

We still need to specify the value of the extrapolation length ξ . We will use an expression due to Zhu, Pine, and Weitz [14],

$$\xi = \frac{2}{3} l \frac{1 + C_2}{1 - C_1}, \quad (21)$$

where the coefficients C_1 and C_2 are the first two moments of $R(\mu)$,

$$C_1 = 2 \int_0^1 d\mu \mu R(\mu), \quad (22a)$$

$$C_2 = 3 \int_0^1 d\mu \mu^2 R(\mu), \quad (22b)$$

normalized such that $C_1 = C_2 = R$ for an angle-independent reflection probability $R(\mu) = R$. Comparison of Eq. (21) with a numerical solution of the Boltzmann equation in a semi-infinite medium by Aronson [8] shows that it accurately describes the length over which the linear density profile extrapolates to zero. The difference is largest for $n = 1$, when Eq. (21) gives $\xi = \frac{2}{3}l$ while the Boltzmann equation gives an extrapolation length of $0.7104l$ which is somewhat larger [1, 7]. The transmittance T_{diff} is compared in Figs. 2 and 3 with the exact T from the Boltzmann equation.

Once the transmittance T for plane-wave illumination as a function of $\mu_{0,\text{vac}} = \cos \theta_{0,\text{vac}}$ is known, one can

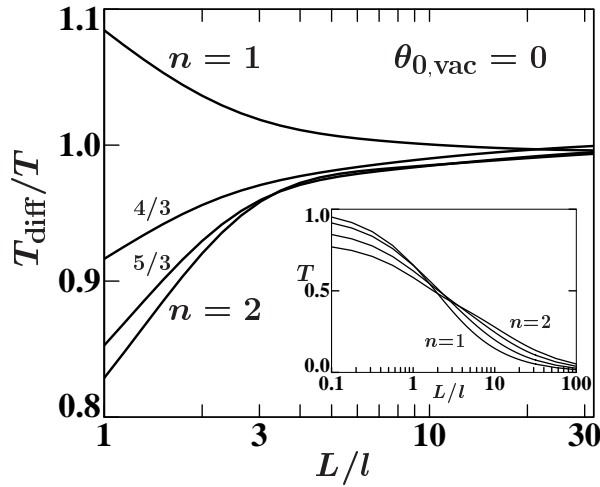


FIG. 3: Ratio of the transmittance T_{diff} according to the diffusion approximation and the exact result T according to the Boltzmann equation, for normal incidence $\theta_{0,\text{vac}} = \theta_0 = 0$. The inset shows T as a function of L/l , for the same values of n as the main plot.

compute the transmittance T_{tot} for diffusive illumination by integrating over the angles of incidence,

$$T_{\text{tot}} = 2 \int_0^1 d\mu_{0,\text{vac}} \mu_{0,\text{vac}} T(\mu_{0,\text{vac}}). \quad (23)$$

The diffusion approximation (20) and (21) yields the an-

alytical formula

$$T_{\text{diff,tot}} = n^2 \left(\frac{3L}{4l} + \frac{1+C_2}{1-C_1} \right)^{-1}. \quad (24)$$

In the absence of a refractive-index mismatch ($n = 1$, $C_1 = C_2 = 0$) this formula has been found [13] to agree with the Boltzmann equation within 3% for all L/l . For $n > 1$ the relative error in Eq. (24) is comparable to that shown in Fig. 3 for the transmittance at normal incidence.

In conclusion, we have computed the transmittance of a turbid medium of mean free path l and length L from the Boltzmann equation as a function of the angle of incidence. We compared the results from the diffusion equation to this exact solution. The difference between the two transmittances stays below 6% for $L > 3l$ and $1 < n < 2$. The diffusion approximation overestimates the transmittance for $n = 1$ and underestimates it in the presence of a significant refractive index mismatch. The relative error is largest for large refractive index mismatch.

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